09/934,972

(FILE 'HOME' ENTERED AT 15:32:35 ON 27 APR 2005)

FILE 'REGISTRY' ENTERED AT 15:33:28 ON 27 APR 2005
L1 STRUCTURE UPLOADED

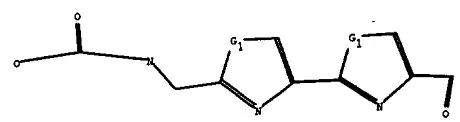
FILE 'STNGUIDE' ENTERED AT 15:33:58 ON 27 APR 2005

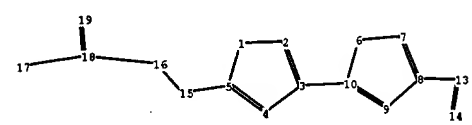
FILE 'REGISTRY' ENTERED AT 15:34:23 ON 27 APR 2005
L2 25 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:35:05 ON 27 APR 2005
L3 13 S L2

=>

C:\Program Files\Stnexp\Queries\





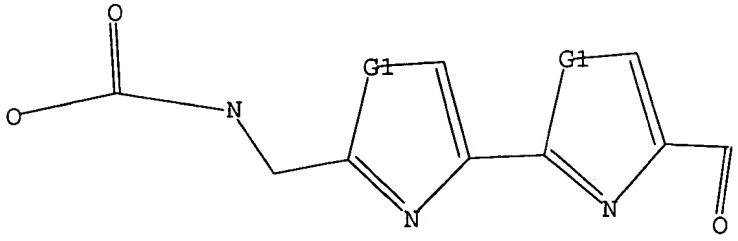
chain nodes :
13 14 15 16 17 18 19
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
3-10 5-15 8-13 13-14 15-16 16-18 17-18 18-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-2 1-5 2-3 3-4 3-10 4-5 5-15 6-7 6-10 7-8 8-9
8-13 9-10 13-14 15-16 16-18 17-18 18-19

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom
8:Atom 9:Atom 10:Atom 13:CLASS 14:CLASS 15:CLASS
16:CLASS 17:CLASS 18:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

L3 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:648054 CAPLUS
DN 132:36007
ED Entered STN: 12 Oct 1999
TI Synthesis of thiazole, imidazole and oxazole containing amino acids for peptide backbone modification
AU Stankova, Ivanka G.; Videnov, Georgi I.; Golovinsky, Evgeny V.; Jung, Guenther
CS Department of Chemistry, Southwest University "N. Rilski", Blagoevgrad, 2700, Bulg.
SO Journal of Peptide Science (1999), 5(9), 392-398
CODEN: JPSIEI; ISSN: 1075-2617
PB John Wiley & Sons Ltd.
DT Journal
LA English
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 28
AB Novel 5-membered heterocyclic ring-containing amino acid building blocks are synthesized. These can be incorporated into analogs of peptide antibiotics such as microcin B17, which is a potent DNA-gyrase inhibitor that exhibits eight thiazole and oxazole moieties. In particular, the syntheses of imidazole and bisoxazole amino acids as novel peptidomimetics are reported, this includes a new procedure for the oxidative conversion of the intermediates oxazoline, imidazoline as well as oxazole-oxazoline into the corresponding heteroarom. compds. A mixture of DBU/CCl4/MeCN and pyridine proved to be a very effective and mild agent for this oxidation step.
ST amino acid heterocyclic prepn peptidomimetic building block; thiazole contg amino acid prepn; imidazole contg amino acid prepn; oxazole contg amino acid prepn; DBU reagent oxazoline oxidn oxazole
IT Amino acids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(heterocyclic; preparation of thiazole, imidazole and oxazole containing amino
acids useful for peptide synthesis)
IT Peptidomimetics
(preparation of thiazole, imidazole and oxazole containing amino acids as building blocks for peptidomimetics)
IT Peptides, preparation
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT Heterocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 84286-90-8P, Microcin B17
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 1113-59-3, 3-Bromo-2-oxopropanoic acid 1138-80-3 1668-10-6, H-Gly-NH2·HCl 5680-80-8, H-Ser-OMe·HCl 161372-39-0 200116-81-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 949-90-6P 1755-98-2P 35150-09-5P 182120-87-2P 252348-72-4P 252348-73-5P 252348-75-7P 252348-77-9P 252348-78-0P 252348-79-1P

252348-80-4P 252348-81-5P **252348-82-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 252348-74-6P 252348-76-8P **252348-83-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(2) Anderson, M; J Chem Soc Perkin Trans 2 1986, P1995 CAPLUS
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(4) Bayer, A; Angew Chem Int Ed Engl 1993, V32, P1336
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(20) Pattenden, G; J Heterocyclic Chem 1992, V29, P607 CAPLUS
(21) Pozdnev, V; Tetrahedron Lett 1995, V36, P7115 CAPLUS
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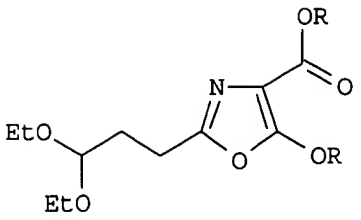
(35) Zhi Ling, Y; J Med Chem 1997, V40, P3297

L3 ANSWER 11 OF 13 CAPLUS
AN 1998:120827 CAPLUS
DN 128:204827
ED Entered STN: 28 Feb 1998
TI Synthesis of functionalized oxazoles and bis-oxazoles
AU Bagley, Mark C.; Buck, Richard T.; Hind, S. Lucy; Moody, Christopher J.
CS Dep. Chem., Univ. Exeter, Exeter, Devon, EX4 4QD, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (3), 591-600
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

OS CASREACT 128:204827

GI



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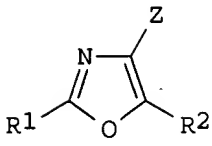
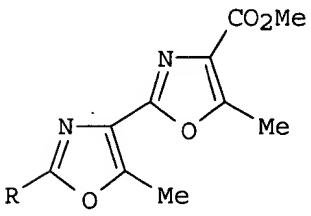
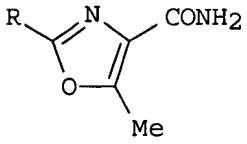


II



III



IV

AB A new method for the synthesis of oxazoles, and in particular chiral non-racemic oxazoles derived from amino acids, has been developed. Thus, rhodium(II) catalyzed reaction of diazocarbonyl compds. RO2CC(CO2R):N2 (R = Me, CMe3) and R2COCZ:N2 (R2 = Me, CH2Cl, Et, Ph, Z = CO2Me, CO2Et) in the presence of amides (EtO)2CHCH2CH2CONH2 and R1CONH2 [R1 = CbzNHCH2, (S)-BocNHCHCHMe2, (S)-CbzNHCHMe, etc.] results in regioselective insertion of the carbenoid into the amide N-H bond with formation of the β-carbonyl amides (EtO)2CH(CH2)2CONHCH(CO2R)2 and R2COCHZNHCOR1, resp. Cyclodehydration of these amides using triphenylphosphine-iodine-triethylamine gives functionalized oxazoles I and II. II [R1 = (S)-CbzNHCHCHMe2, (S)-N-Cbz-pyrrolidin-2-yl, R2 = Me, Z = CO2Me] were converted into the bis-oxazoles III by a second rhodium(II) catalyzed regioselective N-H insertion reaction on the amides IV, followed by cyclodehydration.

ST oxazole prepn; bisoxazole prepn

IT 1138-80-3 1142-20-7 1148-11-4 1149-26-4 6306-54-3 13734-41-3 18381-45-8 25275-28-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxazoles and bis-oxazoles)

IT 949-90-6P 2624-36-4P 6773-29-1P, Dimethyl diazomalonate 13139-27-0P 13139-28-1P 24762-04-7P 28383-65-5P 34079-31-7P 35150-08-4P 35207-75-1P, Di-tert-butyl diazomalonate 104034-82-4P 182866-61-1P 182866-62-2P 182866-63-3P 182866-64-4P 182866-65-5P 182866-66-6P 182866-67-7P 182866-68-8P 182866-71-3P 182866-72-4P 182866-73-5P 182866-74-6P 182866-75-7P 182866-76-8P 203782-20-1P 203782-26-7P 203782-27-8P 203782-28-9P 203782-29-0P 203782-30-3P 203782-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxazoles and bis-oxazoles)

IT 182866-69-9P 182866-70-2P 203782-21-2P 203782-22-3P 203782-23-4P 203782-24-5P 203782-25-6P **203782-32-5P** 203782-33-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of oxazoles and bis-oxazoles)

RE.CNT 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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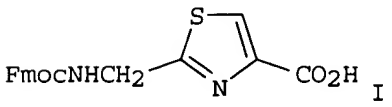
(65) Zaragoza, F; Tetrahedron 1997, V53, P3425 CAPLUS

AN 1996:639425 CAPLUS
DN 125:329404
ED Entered STN: 30 Oct 1996
TI Synthesis of all-thiazole microcin B17
AU Videnov, G.; Ihlenfeldt, H. G.; Bayer, A.; Jung, G.
CS Institut fur Organische Chemie, Universitat Tubingen, Tuebingen, D-72076, Germany
SO Peptides 1994, Proceedings of the European Peptide Symposium, 23rd, Braga, Port., Sept. 4-10, 1994 (1995), Meeting Date 1994, 351-352. Editor(s): Maia, Hernani L. S. Publisher: ESCOM, Leiden, Neth.
CODEN: 63MBAO
DT Conference
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
GI



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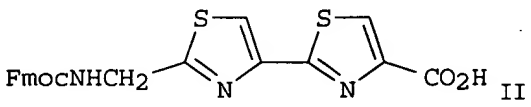
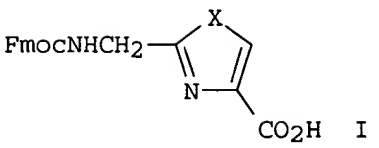


II

AB A report from a symposium on the solid-phase preparation of a microcin B17 analog in which all the oxazole rings are replaced with thiazole rings using thiazole and thoiazolylthiazole building blocks I and II (Fmoc = 9-fluorenylmethoxycarbonyl).
ST Merrifield synthesis thiazole microcin B17 symposium
IT Merrifield synthesis
(solid-phase preparation of all-thiazole microcin B17)
IT 182120-85-0P **182120-86-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of all-thiazole microcin B17)
IT 84286-90-8DP, Microcin B17, all-thiazole analog 183270-54-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase preparation of all-thiazole microcin B17)

L3 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:473413 CAPLUS
DN 125:248418
ED Entered STN: 10 Aug 1996
TI Synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics
AU Videnov, Georgi; Kaiser, Dietmar; Kempter, Christoph; Jung, Guenther
CS Dipl.-Chem. C. Kempter, Inst. Organische Chemie Universitaet, Tuebingen, D-72076, Germany
SO Angewandte Chemie, International Edition in English (1996), 35(13/14), 1503-1506
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 28
OS CASREACT 125:248418
GI



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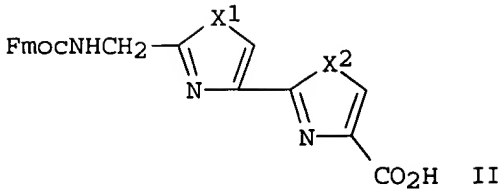

II

AB Oxazole- and thiazole-containing peptides I (X = O, S) and II (X1, X2 = O, S) were prepared starting from glycinamide. Oxidative conversion of intermediate oxazoline into corresponding oxazole was carried out using DBU.

ST peptide mimetic oxazole thiazole

IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

IT 1113-59-3 1668-10-6, Glycinamide hydrochloride 5680-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

IT 35150-09-5P 71904-80-8P 89226-13-1P 182120-82-7P 182120-83-8P
182120-84-9P 182120-87-2P 182120-88-3P 182120-89-4P
182120-90-7P 182120-92-9P 182120-93-0P **182120-94-1P**
182120-95-2P 182120-97-4P 182120-98-5P **182120-99-6P**
182121-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

IT 182120-85-0P **182120-86-1P** 182120-91-8P **182120-96-3P**
182121-01-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

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09/934,972

(FILE 'HOME' ENTERED AT 15:41:25 ON 27 APR 2005)

FILE 'REGISTRY' ENTERED AT 15:41:35 ON 27 APR 2005

L1 STRUCTURE UPLOADED

L2 57 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:42:20 ON 27 APR 2005

L3 80 S L2

L4 3 S L3 AND LIBRAR?

L5 77 S L3 NOT L4

L6 77 DUP REM L5 (0 DUPLICATES REMOVED)

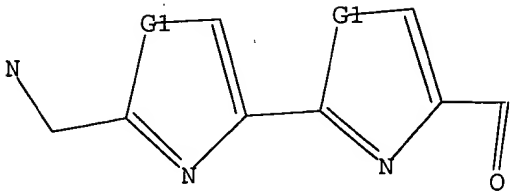
L7 77 S L6

L8 45 S L6 AND PEPTID?

L9 2 S L8 AND COMBINAT?

HAS NO ANSWERS

L1 STR



G1 O,S

09/936,972

(FILE 'HOME' ENTERED AT 15:04:23 ON 27 APR 2005)

FILE 'REGISTRY' ENTERED AT 15:04:40 ON 27 APR 2005

L1 STRUCTURE UPLOADED

L2 1 S L1

FILE 'STNGUIDE' ENTERED AT 15:07:59 ON 27 APR 2005

FILE 'CAPLUS, EMBASE, BIOSIS, MEDLINE, WPIDS' ENTERED AT 15:14:01 ON 27 APR 2005

L3 11526 S (MARTIN, L? OR MARTIN L?)/AU,IN

L4 4515 S (HU, B? OR HU B?)/AU,IN

L5 9 S L3 AND L4

L6 6 DUP REM L5 (3 DUPLICATES REMOVED)

FILE 'STNGUIDE' ENTERED AT 15:16:54 ON 27 APR 2005

FILE 'CAPLUS, EMBASE, BIOSIS, MEDLINE, WPIDS' ENTERED AT 15:20:35 ON 27 APR 2005

L7 3923 S OXAZOLE? AND THIAZOL?

L8 16 S L7 AND PEPTIDOMIMET?

L9 13 DUP REM L8 (3 DUPLICATES REMOVED)

L10 6826 S (JUNG, G? OR JUNG G?)/AU,IN

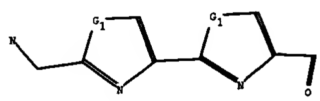
L11 31 S L10 AND OXAZOL?

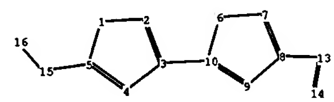
L12 25 S L11 AND THIAZOL?

L13 14 DUP REM L12 (11 DUPLICATES REMOVED)

FILE 'STNGUIDE' ENTERED AT 15:25:10 ON 27 APR 2005

FILE 'CAPLUS, EMBASE, BIOSIS, MEDLINE, WPIDS' ENTERED AT 15:27:57 ON 27 APR 2005





chain nodes :
13 14 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
3-10 5-15 8-13 13-14 15-16
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-2 1-5 2-3 3-4 3-10 4-5 5-15 6-7 6-10 7-8 8-9
8-13 9-10 13-14 15-16

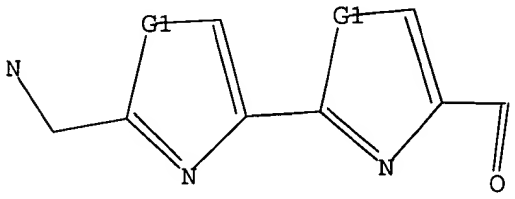
G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom
8:Atom 9:Atom 10:Atom 13:CLASS 14:CLASS 15:CLASS
16:CLASS

Uploading C:\Program Files\Stnexp\Queries\09936972.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 15:05:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9 TO 360
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d all

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 234125-15-6 REGISTRY
ED Entered STN: 21 Aug 1999
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-(aminomethyl)-4-thiazolecarbonylglycylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 36
NTE

type	location		description
uncommon	Oaa-13	-	-
uncommon	Oaa-19	-	-
uncommon	Oaa-21	-	-
uncommon	Oaa-24	-	-
uncommon	Oaa-30	-	-
uncommon	Oaa-32	-	-

SEQ 1 VGIGGGGGGG GGXGGQGGXG XSNXGGGNGX GXGSHI

SEQ3 1 Val-Gly-Ile-Gly-Gly-Gly-Gly-Gly-Gly-Gly-
11 Gly-Gly-Oaa-Gly-Gly-Gln-Gly-Gly-Oaa-Gly-
21 Oaa-Ser-Asn-Oaa-Gly-Gly-Gly-Asn-Gly-Oaa-
31 Gly-Oaa-Gly-Ser-His-Ile

MF C117 H158 N48 O45 S4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3N2	NCNC2	5	C3N2	16.195.24	1
C3NO	NCOC2	5	C3NO	16.239.9	3
C3NS	NCSC2	5	C3NS	16.299.11	4

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 135:269150 CA
TI In vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bisheterocyclic sites
AU Zamble, Deborah B.; Miller, Deborah A.; Heddle, Jonathan G.; Maxwell, Anthony; Walsh, Christopher T.; Hollfelder, Florian
CS Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SO Proceedings of the National Academy of Sciences of the United States of America (2001), 98(14), 7712-7717
CODEN: PNASA6; ISSN: 0027-8424
PB National Academy of Sciences
DT Journal
LA English
CC 7-3 (Enzymes)
AB Microcin B17 (MccB17) is a 3.1-kDa Escherichia coli antibiotic that contains thiazole and oxazole heterocycles in a peptide backbone. MccB17 inhibits its cellular target, DNA gyrase, by trapping the enzyme in a complex that is covalently bound to double-strand cleaved DNA, in a manner similar to the well-known quinolone drugs. The identification of gyrase as the target of MccB17 provides an opportunity to analyze the relationship between the structure of this unusual antibiotic and its activity. In this report, steady-state parameters are used to describe the induction of the cleavable complex by MccB17 analogs containing modified bis-heterocyclic sites. The relative potency of these analogs corresponds to the capacity of the compds. to prevent growth of sensitive cells. In contrast to previously reported expts., inhibition of DNA gyrase supercoiling activity by wild-type MccB17 also was observed These results suggest that DNA gyrase is the main intracellular target of MccB17. This study probes the structure-function relationship of a new class of gyrase inhibitors and demonstrates that these techniques could be used to analyze compds. in the search for clin. useful antibiotics that block DNA gyrase.
ST DNA gyrase inhibition microcin B17 analog
IT Enzymes, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(DNA gyrases, A and B; in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
IT Structure-activity relationship
(enzyme-inhibiting, DNA gyrase-inhibiting; in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
IT Enzyme kinetics
Supercoiled structure
(in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
IT 84286-90-8, microcin B17 84286-90-8D, microcin B17, analogs 234125-07-6 234125-08-7 234125-11-2 234125-15-6 234125-18-9
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Bayer, A; Eur J Biochem 1995, V234, P414 CAPLUS
(2) Critchlow, S; Biochemistry 1996, V35, P7387 CAPLUS
(3) Drlica, K; Curr Opin Microbiol 1999, V2, P504 CAPLUS
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(25) Yorgey, P; Proc Natl Acad Sci USA 1994, V91, P4519 CAPLUS
(26) Yoshida, H; Antimicrob Agents Chemother 1993, V37, P839 CAPLUS
(27) Zuber, G; J Am Chem Soc 1998, V120, P9368 CAPLUS

REFERENCE 2

AN 131:127509 CA
TI In vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites
AU Roy, Ranabir Sinha; Kelleher, Neil L.; Milne, Jill C.; Walsh, Christopher T.
CS Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SO Chemistry & Biology (1999), 6(5), 305-318
CODEN: CBOLE2; ISSN: 1074-5521
PB Current Biology Publications
DT Journal
LA English
CC 10-5 (Microbial, Algal, and Fungal Biochemistry)

AB The Escherichia coli peptide antibiotic microcin B17 (MccB17) contains 4 oxazole and 4 thiazole rings and inhibits DNA gyrase. The role of individual and tandem pairs of heterocycles in bioactivity has not been determined previously. The 2 tandem 4,2-bisheterocycles in MccB17 were varied by expression of MccB17 or mutants containing altered sequences at Gly39-Ser40-Cys41 or Gly54-Cys55-Ser56. A mixture of 5-9-ring MccB17 isoforms were separated and quantitated for antibiotic potency. Mutagenesis of the thiazole-oxazole pair significantly affected antibiotic activity compared with the upstream oxazole-thiazole, which might stabilize partially cyclized intermediates against proteolysis. Enzymic heterocyclization in native MccB17 occurs distributively. Antibiotic activity correlates with the number of rings and is differentially sensitive to both the location and the identity of the 4,2-tandem heterocycle pairs in MccB17. Such tandem heterocycles might be useful pharmacophores in combinatorial libraries.

ST antibiotic activity microcin B17 analog

IT Structure-activity relationship
(bactericidal; in vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites)

IT Antibiotics
(in vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites)

IT 84286-90-8DP, Microcin B17, analogs 234125-07-6P 234125-08-7P 234125-09-8P 234125-10-1P 234125-11-2P 234125-12-3P 234125-13-4P 234125-14-5P 234125-15-6P 234125-16-7P 234125-17-8P 234125-18-9P
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)
(in vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites)

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD

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=>

L13 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:639425 CAPLUS
DN 125:329404
TI Synthesis of all-**thiazole** microcin B17
AU Videnov, G.; Ihlenfeldt, H. G.; Bayer, A.; **Jung, G.**
CS Institut fur Organische Chemie, Universitat Tubingen, Tuebingen, D-72076, Germany
SO Peptides 1994, Proceedings of the European Peptide Symposium, 23rd, Braga, Port., Sept. 4-10, 1994 (1995), Meeting Date 1994, 351-352. Editor(s): Maia, Hernani L. S. Publisher: ESCOM, Leiden, Neth.
CODEN: 63MBAO
DT Conference
LA English

L13 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:288460 CAPLUS
DN 133:4987
ED Entered STN: 04 May 2000
TI Synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides, cyclotetrapeptide and their antibacterial activity in vitro
AU Stankova, Ivanka G.; Videnov, Georgi I.; Tabakova, Svoboda; Golovinsky, Evgeny V.; **Jung, Guenther**
CS Department of Chemistry, South - West University "N. Rilski", Blagoevgrad, 2700, Bulg.
SO Peptides 1998, Proceedings of the European Peptide Symposium, 25th, Budapest, Aug. 30-Sept. 4, 1998 (1999), Meeting Date 1998, 248-249. Editor(s): Bajusz, Sandor; Hudecz, Ferenc. Publisher: Akademiai Kiado, Budapest, Hung.
CODEN: 68WKAY
DT Conference
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 10, 28
AB A symposium report. We describe the synthesis and antibacterial activity of new peptides and a cyclopeptide containing imidazole, **thiazole** and **oxazole** rings. Two compds. were active against Staphylococcus, Klebsiella and Streptococcus strains.
ST peptide imidazole **thiazole** **oxazole** ring prepn antibacterial symposium
IT Antibacterial agents
(synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides and a cyclotetrapeptide and their antibacterial activity in vitro)
IT Peptides, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides and a cyclotetrapeptide and their antibacterial activity in vitro)
IT 270908-01-5P 270908-02-6P 270908-03-7P 270908-04-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides and a cyclotetrapeptide and their antibacterial activity in vitro)
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Bergeron, J; J Org Chem 1985, V50, P2780
(2) Fusetani, N; Chem Rev 1993, V93, P1793 CAPLUS
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